1,3-diphenylpropane-1,2-diol 5381-84-0 | DTXSID50281584

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 12.2 days

Global applicability domain: Outside

Local applicability domain index: 3.28e-01

Confidence level: 8.62e-01

Nearest Neighbors from the Training Set

Image not found

9-Ethyl-9H-fluorene Measured: 2330 Predicted: N/A Image not found

2-Methylphenanthrene Measured: 1370 Predicted: 25.0 Image not found

5-Methylindan Measured: 4.93 Predicted: 2.25

Image not found

Phenanthrene, trimethyl-Measured: 26200 Predicted: 75.6 Image not found

4-Methylindan Measured: 4.93 Predicted: 2.31